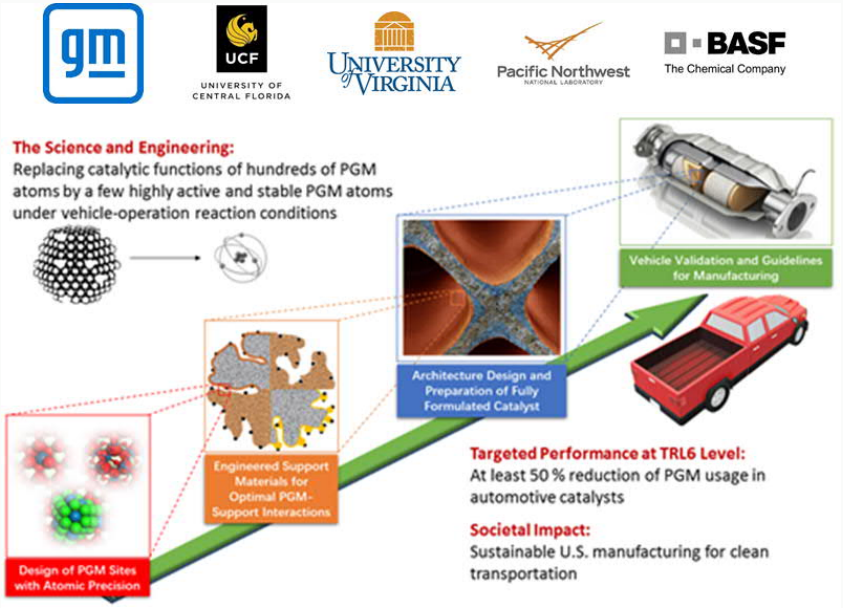


Slashing PGM in Catalytic Converters: An Atoms-to-Autos Approach

Wei Li, General Motors
Annual Merit Review (ACE 158)
6/21/2022

PGM: Platinum Group Metals

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Overview

Timeline

- Start – October 2020
- Finish – December 2023
- 40% Complete

Funding

- Project Budget $3.35 million
  - $1.75M Federal Share
  - $1.60M Cost Share
- 2021 funds received $113,439
- 2022 funding planned $595,213

Vehicle Technology Barriers

- Low temperature emission performance
- High PGM loadings
- PGM sintering

Project Team

- General Motors, LLC
- Pacific Northwest National Lab
- University of Central Florida
- University of Virginia
- BASF Corporation

general motors

Acknowledgment: This material is based upon work supported by the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy (EERE) under the Vehicle Technologies Program Office Award Number DE-EE0009196.

Relevance

- Global demand for PGM is outstripping supply, driven by
  - increasing global production of vehicles with internal combustion engines
  - increasingly stringent emissions standards
  - higher emission control system durability requirements
- Overall Project Objectives
  - Develop catalysts with predominantly single-atoms or small ensembles to identify the most promising Pd and Rh structures for TWC catalysts

This atoms-to-autos approach aims to reduce PGM use in the U.S. vehicle fleet by 50% while meeting future emission regulations (including SULEV30)

Technical Approach

- Overall Approach
  - Improve the utilization efficiency of PGMs in gasoline TWCs by engineering PGM sites and support materials with near 100% metal dispersion
  - *Uses PGM single atoms as building blocks, not necessarily as final catalytic centers*
  - Material development effort will be supported by detailed kinetic studies and advanced characterization tools
  - Individual Pd and Rh catalysts with scalable preparation methods; rational washcoat structure design for integration and full-size validation
- 2021 Task Plan
  - Baseline catalyst technology definition (completed)
  - Design Pd and Rh Catalysts with Near 100% Material Efficiency and Optimal Catalytic Activities and Durability (completed)
  - End-of-year Goal: Downselection of Technology Pathway for Individual Pd and Rh Catalysts (completed)

Technical Accomplishments

Baseline Catalyst Technology Defined

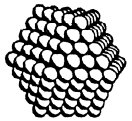
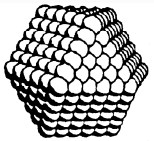
- 2020 GM vehicle with turbo-charged 2L engine
- Baseline Pd and Rh Catalysts
- Aging and Test Conditions (LTAT protocols):
  - *Degreen: 700°C hydrothermal 2 hours*
  - *Aging: lean-rich 950°C for 50 h*
  - *Powder samples degreened and aged at GM and distributed to team members: consistent baseline*

Table 1: Lab reactor test feed concentrations λ = 0.995

$[C_3H_6]$	$[C_3H_8]$	[CO]	$[H_2]$	[NO]	$[O_2]$	$[CO_2]$	$[H_2O]$
666 ppm	333 ppm	5000 ppm	1700 ppm	1000 ppm	6400 ppm	13%	13%

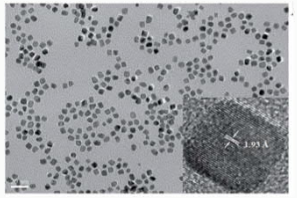
What are Single Atom Catalysts?

Increasing utilization

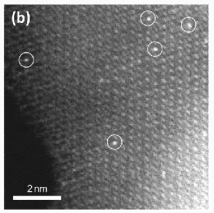
Full-Shell "Magic Number" Clusters					
Number of shells	1	2	3	4	5
Number of atoms in cluster	M_{13}	M_{55}	M_{147}	M_{309}	M_{561}
Percentage surface atoms	92%	76%	63%	52%	45%

Chen *et al.* Surf. Sci. Rep. 2019, 74, 100471

Pt Black



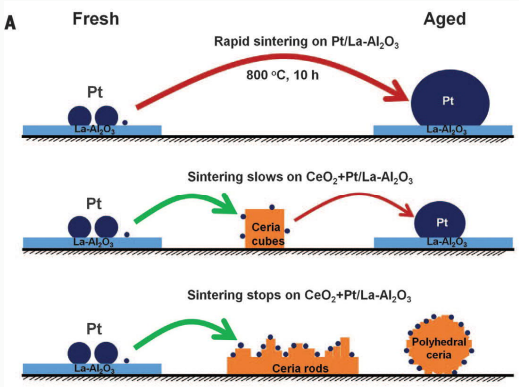
Pt Nanoparticles

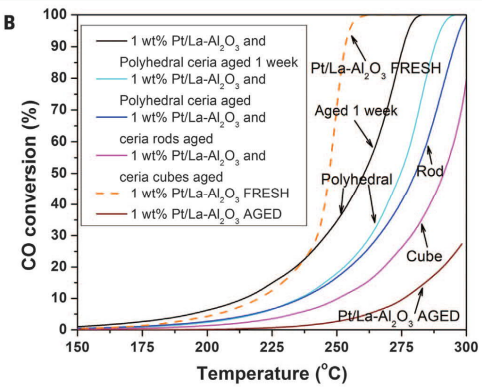


Pt atom

Increasing utilization

Yang *et al.* Acc. Chem. Res. 2013, 46, 8, 1740-1748

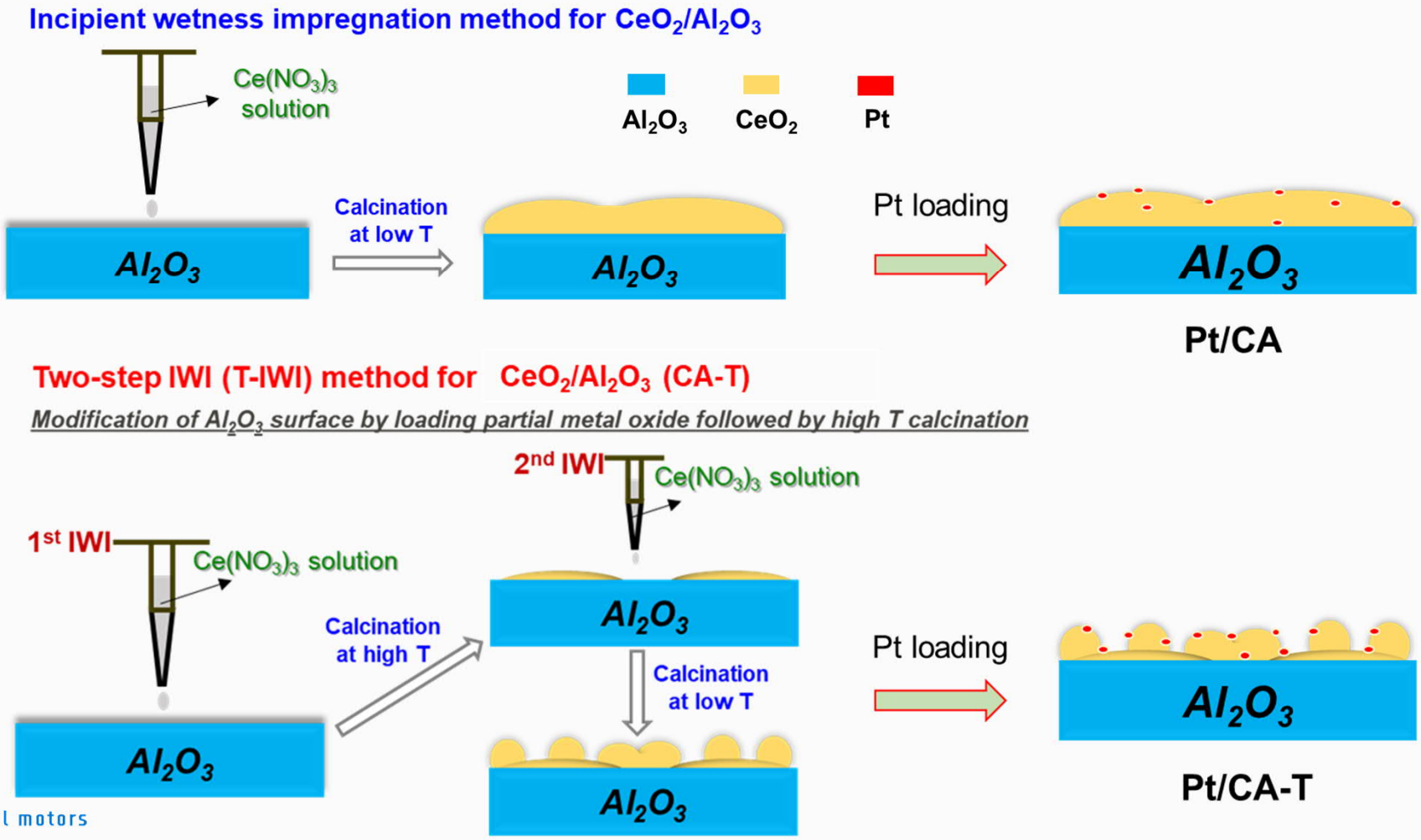




Jones *et al*. Science 353 (6295), 150-154, 2016

- Single atom catalysts (SACs) offer potential 100% atomic efficiency
- SACs have well-defined active centers that may be tuned for high activities and selectivities.
- Durability of SACs under realistic engine exhaust conditions is a significant technical challenge

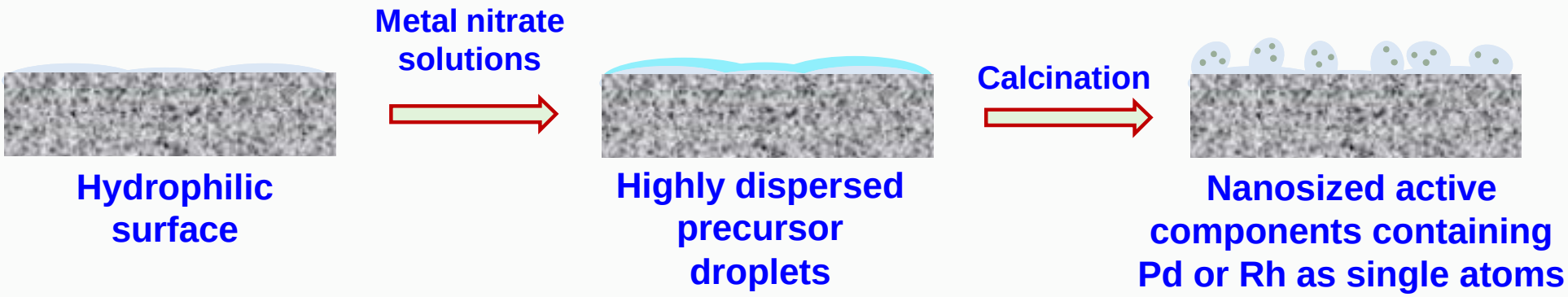
Support Surface Modification Strategy



Xie, Liu *et al.* ***J. Catal.*** 2022, 405, 236-248.

New Concept for DOE TWC Project

Creating active Pd, Rh single atom species on hydrophilic support

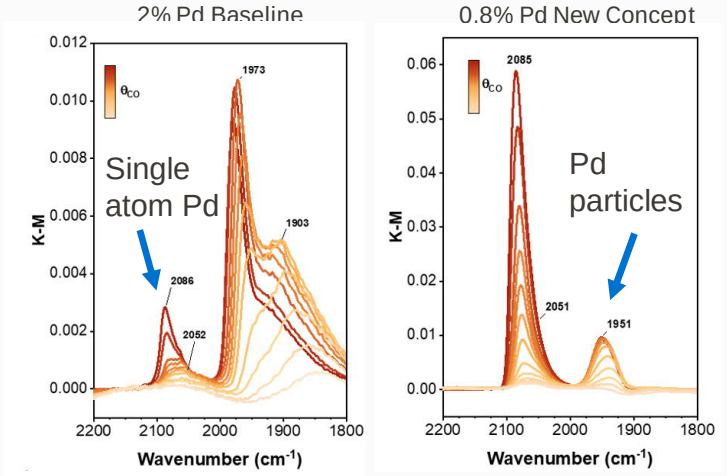


- Pd and Rh species present as single atoms or small clusters in the fresh state, close to 100% dispersion.
- Engineered supports provide anchoring sites for improved thermal durability

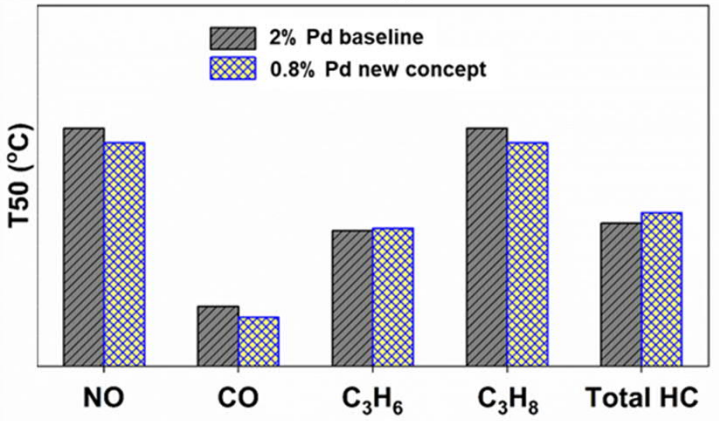
Palladium Single Atom Catalyst Development

- Palladium single atom catalysts prepared and confirmed by infrared spectra after CO adsorption
- Preparation method optimized to tune the Pd-support surface interaction:
  - Alumina support properties
  - Cerium precursors
  - Promoters and loadings
  - Calcination temperatures
- With 60% reduction of Pd usage, 0.8% Pd new concept catalyst showed TWC activities comparable to the 2% Pd baseline after lean-rich aging at 950°C.

Infrared Spectra of CO adsorption



Lab Reactor TWC Lightoff Test Results

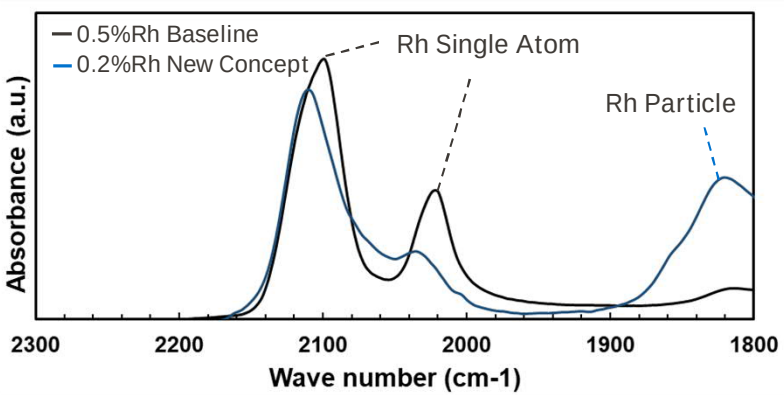


T50: temperature at 50% conversion

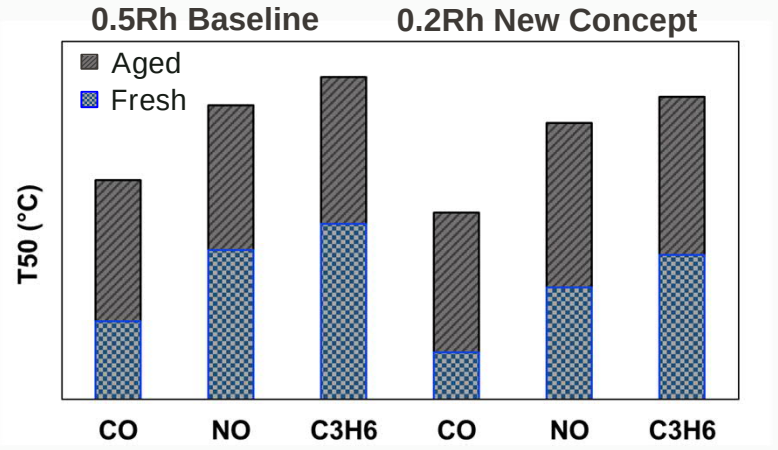
Rhodium Single Atom Catalyst Development

- Rhodium single atom catalysts prepared and confirmed by infrared spectra after CO adsorption
- Preparation method optimized:
  - Alumina support properties
  - Cerium precursors
  - Promoters and loadings
  - Calcination temperatures
- With 60% reduction of Rh usage, 0.2wt.% Rh new concept catalyst showed TWC activities comparable to the 0.5wt.% baseline after lean-rich aging at 950°C.

Infrared Spectra of CO adsorption



Lab Reactor TWC Lightoff Test Results



T50: temperature at 50% conversion

2021/2022 Milestones

Budget Period	Milestone	Description	Milestone or Go/No-Go Decision	Status
1	1.1	Definition of catalyst systems and experimental protocols	Milestone	Completed
	1.2	Evaluation of Pd and Rh species and support materials	Milestone	Completed
	1.3	Desired optimal Pd, Rh species and supports identified and prepared	Milestone	Completed
	1.4	Proof of design concept to achieve performance measures	Go/No-Go Decision	Completed
2	2.1	Optimal supported Pd and Rh catalysts developed and prepared	Milestone	On track
	2.2	Pd and Rh species optimized for aged performance	Milestone	On track
	2.3	Optimized Pd and Rh catalysts after aging validated in core samples	Milestone	Not started
	2.4	Design concept optimized and aged performance validated	Go/No-Go Decision	N/A

Collaborations

- **BASF** (*Yuejin Li, Xiaolai Zheng*)
  - Baseline catalysts (powder, core)
  - Catalyst scale-up and washcoat design; full-size part preparation
- **University of Central Florida** (*Prof. Fudong Liu*)
  - Support engineering
  - Single-atom catalyst development
- **University of Virginia** (*Prof. Bill Epling*)
  - Catalyst aging study
  - Reaction kinetics and mechanism
- **Pacific Northwest National Lab** (*Ken Rappe, Nick Nelson*)
  - Catalyst characterization
- **General Motors** (*Wei Li, Kevin Gu*)
  - Overall project management
  - Single-atom catalyst development; system level demonstration

Proposed Future Research

- *Budget Period Two (1/2022 – 12/2022): on-going*
  - Concurrent optimization of the Pd and Rh species and the engineered supports
  - Demonstrate ≥60% PGM cost reduction in core sample form
- *Budget Period Three (1/2023 – 12/2023):*
  - Transform powder and core samples to full-size, fully formulated catalysts
  - Demonstrate pathway to 50% PGM cost savings on engine dynamometer or vehicle

Any proposed future work is subject to change based on funding levels.

Summary

- Extensive collaboration among the team partners
- Identified technical pathway:
  - Single atoms and small ensembles
  - Engineered supports
- Budget period one milestones achieved (60% Pd/Rh reduction at powder level lab testing)
  - 0.8 wt.% Pd catalyst equivalent performance with baseline 2 wt.% Pd
  - 0.2 wt.% Rh catalyst equivalent performance with baseline 0.5 wt.% Rh